

Self-energy approach to the correlated Kondo-lattice model

W. Nolting^a, G. G. Reddy^b, A. Ramakanth^b, D. Meyer^c, and J. Kienert^a

^a *Lehrstuhl Festkörpertheorie, Institut für Physik, Humboldt-Universität zu Berlin, Invalidenstr. 110, 110115 Berlin, Germany*

^b *Kakatiya University, Department of Physics, Warangal-506009, India*

^c *Department of Mathematics, Imperial College, 180 Queen's Gate, London SW7 2BZ, United Kingdom*

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We develop an interpolating self-energy approach to the correlated Kondo-lattice model. The correlation of the band electrons is taken into account by a Hubbard interaction. The method is based on a self-energy ansatz, the structure of which allows to fulfill a maximum number of exactly solvable limiting cases. The parameters of the ansatz are fitted to spectral moments via high-energy expansion of the self-energy. The band electron correlations are taken into account by an effective medium approach being correct in the strong coupling (U) regime. The theory is considered reliable for all temperatures, band occupations, and exchange couplings. Results are presented for the respective dependencies of spectral densities, quasiparticle densities of states, and characteristic correlation functions, and interpreted in terms of elementary spin exchange processes between itinerant conduction electrons and localized magnetic moments. The appearance of magnetic polarons, the typical quasiparticle of Kondo-lattices, in the energy spectrum is worked out. Spin exchange processes prevent a total spin polarization of the band electrons even for arbitrarily strong exchange couplings as long as the local moments are represented by quantum mechanical spins.

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I. INTRODUCTION

The Kondo-lattice model (KLM)^{1,2,3,4,5,6,7} is surely one of the most intensively discussed models in solid state theory. It aims at the mutual influence of two electronic subsystems. The one consists of itinerant particles in a partially filled energy band, the other is built up by at certain lattice sites strictly localized electrons. The latter give rise to permanent magnetic moments which are described as quantum mechanical spins. Characteristic model properties result from an interband exchange, which is written as an intra-atomic interaction of strength J between the conduction electron spin σ_i and local-moment spin \mathbf{S}_i :

$$H_{sf} = -J \sum_i \sigma_i \cdot \mathbf{S}_i. \quad (1)$$

The index i refers to the lattice site \mathbf{R}_i . According to the sign of the exchange coupling J , a parallel ($J>0$) or an antiparallel ($J<0$) alignment of itinerant and localized spin is favoured with remarkable differences in the physical properties. We restrict our considerations in the following to the $J>0$ -case, sometimes referred to as *ferromagnetic Kondo-lattice model* (*s-f*, *s-d* model), or, in the strong-coupling regime, as *double-exchange model*.

The interest in the KLM explains itself by rather manifold applications. There are mainly four groups of materials, the fundamental properties of which are considered to be well-described by the exchange (1):

- (a) (Concentrated) magnetic semiconductors EuO, EuS, ..
- (b) Local-moment metals Gd, Tb, Dy, $\text{Eu}_{1-x}\text{Gd}_x\text{S}$, ..

- (c) Diluted magnetic semiconductors (DMS) $\text{Ga}_{1-x}\text{Mn}_x\text{As}$, ..

- (d) Manganites (colossal magneto-resistance materials, CMR) $\text{La}_{1-x}(\text{Ca}, \text{Sr})_x\text{MnO}_3$

The rich variety of hot topics in solid state theory, being related to the KLM, deserves a reliable approach to this not exactly solvable many-body problem. Most of recent theoretical works on the KLM, aiming predominantly at the CMR-materials, assume classical spins ($S \rightarrow \infty$).^{8,9,10} However, this seems to be a rather questionable starting point, only *justified* by the fact that then *dynamical mean field theory* (DMFT) can be applied. Characteristic features such as magnon emission (absorption) of the conduction electron are ruled out from the very beginning. The same holds for the formation of *magnetic polarons*, the characteristic quasiparticles of Kondo-lattices. The importance of such effects can impressively be demonstrated by the exactly solvable limiting case of a single electron in an otherwise empty conduction band, interacting with a ferromagnetically saturated spin system^{11,12} (see Figs. 1, 2 in Ref. 13). Recently we proposed a DMFT-based approach to the KLM with quantum spins using a fermionization of the local spin operators ($S=1/2$). Even for rather moderate exchange coupling an unusual quasiparticle structure appears due to the above-mentioned elementary processes. The results are in remarkable agreement with those from the *moment conserving decoupling approach* (MCDA), introduced in Ref. 14 and successfully applied to several topics in previous papers.^{15,16,17,18,19,20} The MCDA as well as the DMFT-based approach are both considered to work in the low and intermediate coupling regime,¹³ therefore suitable for modelling systems such as EuO, EuS, Gd.^{15,16,17,19} For strongly coupled systems (DMS, CMR-materials) with finite band occupations alterna-

tives are desirable. Very recently the authors have presented a self-energy approach which interpolates between a maximum number of exactly solvable limiting cases.²¹ On the one hand, it should be a reasonable ansatz for weak as well as strong couplings, on the other hand, however, it represents a low-density approach, strictly justified for $n \rightarrow 0$ only. We are going to present in this paper a new and extended ansatz, which is considered to work for all couplings and all band occupations reasonably well. For $n \rightarrow 0$ it turns out to be identical to the ansatz in Ref. 21.

The inclusion of finite band occupations provokes some non-trivial problems. First, some physically important correlation functions appear, which have to be determined self-consistently via spectral theorem and properly defined *higher* Green functions. These are, in particular, *mixed* correlations, i.e. averages of products of local spin operators with band electron operators. More fundamental, however, is another point: In the *normal* KLM the band electrons are considered as uncorrelated particles. It can be shown, directly to be seen in the exact zero-bandwidth limit,²² that the transition from a single- to a double-occupied site can unphysically be connected with a gain in energy. In reality, the Coulomb repulsion will rather block such double occupancies. To guarantee this in the model, too, we shall add to the *normal* KLM an intra-atomic Coulomb interaction as has been proposed in Ref. 10. One then speaks of the *correlated Kondo-lattice model* (CKLM).

In Sec. II we first formulate in detail the Hamiltonian of the CKLM and its many-body problem. Furthermore, we list up some rigorous facts which are used in Sec. III to create an interpolation formula for the electronic self-energy. This interpolation scheme is the crucial point of our procedure. The resulting data are finally discussed in Sec. IV, mainly in terms of spectral densities (SD) and quasiparticle densities of states (QDOS). The above-mentioned rigorous facts have partly been presented already in our preceding paper.²¹ So we restrict the presentation to the points which are vital for the understanding of the following theory and the subsequent discussions.

II. THEORY

A. The many-body problem

The Hamiltonian of the *correlated Kondo-lattice model* (CKLM) consists of three partial operators:

$$H = H_S + H_U + H_{sf}. \quad (2)$$

H_S is the kinetic energy of itinerant band electrons:

$$H_S = \sum_{ij\sigma} (T_{ij} - \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} = \sum_{\mathbf{k}\sigma} (\epsilon(\mathbf{k}) - \mu) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \quad (3)$$

T_{ij} are the hopping integrals being connected by Fourier transformation to the *free* Bloch energies $\epsilon(\mathbf{k})$. μ is the

chemical potential. $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) and $c_{\mathbf{k}\sigma}^\dagger$ ($c_{\mathbf{k}\sigma}$) are the creation (annihilation) operators of a conduction electron with spin σ ($\sigma = \uparrow, \downarrow$) at lattice site \mathbf{R}_i and with wavevector \mathbf{k} , respectively.

H_U is an intra-atomic Coulomb interaction of Hubbard-type with the Coulomb-matrix element U :

$$H_U = \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}. \quad (4)$$

$n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the occupation number operator.

Most important is H_{sf} , already introduced by (1). However, better tractable is the second quantized form of the exchange interaction:

$$H_{sf} = -\frac{1}{2} J \sum_{j\sigma} (z_\sigma S_j^z n_{j\sigma} + S_j^{-\sigma} c_{j-\sigma}^\dagger c_{j\sigma}). \quad (5)$$

Here we have written for abbreviation:

$$z_\sigma = \delta_{\sigma\uparrow} - \delta_{\sigma\downarrow}; \quad S_j^\sigma = S_j^x + i z_\sigma S_j^y. \quad (6)$$

The first term in (5) describes an Ising-like interaction between the z -components of the localized and the itinerant spins. The second term is responsible for spin exchange processes between the two subsystems.

Since we are mainly interested in the conduction electron properties, we try to calculate the single electron Green function, from which we can derive all required information. A formal solution for the \mathbf{k} -dependent single-electron Green function can be written as follows:

$$G_{\mathbf{k}\sigma}(E) = \left\langle \left\langle c_{\mathbf{k}\sigma}; c_{\mathbf{k}\sigma}^\dagger \right\rangle \right\rangle_E = \frac{\hbar}{E + \mu - \epsilon(\mathbf{k}) - \Sigma_{\mathbf{k}\sigma}(E)}. \quad (7)$$

The self-energy $\Sigma_{\mathbf{k}\sigma}(E)$ is composed of two parts:

$$\Sigma_{\mathbf{k}\sigma}(E) = \Sigma_{\mathbf{k}\sigma}^{(U)}(E) + \Sigma_{\mathbf{k}\sigma}^{(sf)}(E). \quad (8)$$

The two self-energy parts are defined by the following relation:

$$\left\langle \left\langle [H_{U(sf)}, c_{\mathbf{k}\sigma}]_-; c_{\mathbf{k}\sigma}^\dagger \right\rangle \right\rangle \equiv \Sigma_{\mathbf{k}\sigma}^{(U,sf)}(E) G_{\mathbf{k}\sigma}(E). \quad (9)$$

$[\dots]_{-(+)}$ denotes the (anti)commutator. In general $\Sigma_{\mathbf{k}\sigma}(E)$ will be a complex quantity. It contains all the influences of the various interaction processes being therefore of fundamental importance. To have found $\Sigma_{\mathbf{k}\sigma}(E)$ means to have solved the problem.

Another decisive quantity is the spectral density,

$$S_{\mathbf{k}\sigma}(E) = -\frac{1}{\pi} \text{Im} G_{\mathbf{k}\sigma}(E), \quad (10)$$

which is directly related to the bare lineshape of an angle- and spin-resolved (inverse) photoemission experiment. Additional angle averaging then leads to the quasiparticle density of states:

$$\rho_\sigma(E) = \frac{1}{N\hbar} \sum_{\mathbf{k}} S_{\mathbf{k}\sigma}(E - \mu). \quad (11)$$

We are going to present our results for the CKLM mainly in terms of spectral densities and quasiparticle densities of states.

B. Effective medium approach

Our study is predominantly focussed on the influence of the interband exchange (5) on the conduction band states. As explained in Sec. I the introduction of H_U shall first of all avoid unphysical double occupancies as energetically favoured configurations. For this purpose we assume:

$$U \gg W, J. \quad (12)$$

W is the bandwidth. In this limit the energy band is split for $J=0$ into two quasiparticle subbands. The (\mathbf{k}, σ) -dependent spectral density consists of two peaks centred at^{23,24,25}

$$T_{1\sigma}(\mathbf{k}) = T_0 + (1 - n_{-\sigma})(\epsilon(\mathbf{k}) - T_0) + n_{-\sigma}B_{-\sigma}, \quad (13)$$

$$T_{2\sigma}(\mathbf{k}) = T_0 + U + n_{-\sigma}(\epsilon(\mathbf{k}) - T_0) + (1 - n_{-\sigma})B_{-\sigma}. \quad (14)$$

To the same order, the area under the peaks (*spectral weight*) is given by:

$$\hat{\alpha}_{1\sigma}(\mathbf{k}) = 1 - n_{-\sigma} = 1 - \hat{\alpha}_{2\sigma}(\mathbf{k}). \quad (15)$$

$B_{-\sigma}$ is a higher correlation function, which, however, can exactly be expressed by the spectral density itself:²⁵

$$\begin{aligned} B_{\sigma} &= \frac{1}{n_{\sigma}(1 - n_{\sigma})} \frac{1}{N} \sum_{ij}^{i \neq j} T_{ij} \langle c_{i\sigma}^{\dagger} c_{j\sigma} (2n_{i-\sigma} - 1) \rangle \\ &= \frac{1}{n_{\sigma}(1 - n_{\sigma})} \frac{1}{N} \sum_{\mathbf{k}} [\epsilon(\mathbf{k}) - T_0] \\ &\quad \times \int_{-\infty}^{+\infty} dE f_{-}(E) S_{\mathbf{k}\sigma}^{*}(E - \mu) \left\{ \frac{2}{U} [E - \epsilon(\mathbf{k})] - 1 \right\}. \end{aligned} \quad (16)$$

$S_{\mathbf{k}\sigma}^{*}(E)$ is, at first, the spectral density for the *pure* Hubbard model; however, it will later be changed into the spectral density of the full model to guarantee self-consistency.

In order to account for the Hubbard part H_U in the strong coupling regime we perform an effective medium approach by replacing the single-particle energies in Eq. (3) by the quasiparticle energies (13) and (14), respectively. This means for the Green function (7):

$$G_{\mathbf{k}\sigma}(E) = \sum_{i=1}^2 G_{\mathbf{k}\sigma}^{(i)}(E), \quad (17)$$

$$G_{\mathbf{k}\sigma}^{(i)}(E) = \hbar \frac{\hat{\alpha}_{i\sigma}(\mathbf{k})}{E + \mu - T_{i\sigma}(\mathbf{k}) - \Sigma_{\mathbf{k}\sigma}^{(i)}(E)}. \quad (18)$$

The CKLM has therefore become a *normal* KLM in an effective medium, which is characterized by two (!) energy bands according to the single-particle energies $T_{1,2\sigma}(\mathbf{k})$. The partial self-energies $\Sigma_{\mathbf{k}\sigma}^{(1,2)}(E)$ are formally determined by the interband-exchange, only.

We are left with the many-body problem of the KLM which, for the general case, cannot be treated rigorously either. However, some important facts are known, which can help to find a trustworthy approach.

C. Zero-bandwidth limit

For a self-energy approach that is credible in the strong coupling region ($JS \gg W$) the exactly calculable zero-bandwidth limit²² should be fulfilled:

$$T_{ij} \rightarrow T_0 \delta_{ij} ; \quad \epsilon(\mathbf{k}) \rightarrow T_0 \quad \forall \mathbf{k}. \quad (19)$$

The *free* conduction band is shrunk to an N -fold degenerate level T_0 . This means for the effective medium:

$$T_{1\sigma}(\mathbf{k}) \rightarrow T_0 ; \quad T_{2\sigma}(\mathbf{k}) \rightarrow T_0 + U. \quad (20)$$

To have a physically reasonable limit, however, the localized spin system is furtheron considered as collectively ordered for temperatures $T < T_c$ by any kind of exchange interaction. The respective magnetization $\langle S^z \rangle$ has to be considered as an external parameter. The partial self-energies as defined in (18) read²²

$$\Sigma_{\sigma}^{(1)(W=0)}(E) = \frac{1}{2} J \frac{\frac{1}{2} JS(S+1) - X_{-\sigma}(E + \mu - T_0)}{E + \mu - T_0 - \frac{1}{2} J(1 + X_{-\sigma})}, \quad (21)$$

$$\Sigma_{\sigma}^{(2)(W=0)}(E) = \frac{1}{2} J \frac{\frac{1}{2} JS(S+1) + Y_{-\sigma}(E + \mu - T_0 - U)}{E + \mu - T_0 - U + \frac{1}{2} J(1 + Y_{-\sigma})}. \quad (22)$$

Here we have introduced:

$$X_{\sigma} = \frac{\Delta_{\sigma} - m_{\sigma}}{1 - n_{\sigma}} \quad , \quad Y_{\sigma} = \frac{\Delta_{\sigma}}{n_{\sigma}} \quad , \quad (23)$$

where

$$m_{\sigma} = z_{\sigma} \langle S^z \rangle \quad , \quad \Delta_{\sigma} = \langle S_i^{\sigma} c_{i-\sigma}^{\dagger} c_{i\sigma} \rangle + z_{\sigma} \langle S_i^z n_{i\sigma} \rangle. \quad (24)$$

D. Magnetic polaron

There is another very instructive limiting case that can be solved rigorously.^{11,12} It concerns a single electron (hole) in an otherwise empty (fully occupied) energy band interacting with a ferromagnetically saturated spin system. The details of the derivation of the self-energy can be found in Ref. 26. If we introduce the *effective medium propagators* ($i=1,2$)

$$G_{i\sigma}(E) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\hbar}{E + \mu - T_{i\sigma}(\mathbf{k})} \quad (25)$$

then we have the following $T=0$ -expressions for the self-energy, which are exact for arbitrary bandwidth, coupling, and spin:

$$\begin{aligned} \Sigma_{\mathbf{k}\sigma}^{(n=0)}(E) &\equiv \Sigma_{\sigma}^{(1)(n=0)}(E) \\ &= -\frac{1}{2} z_{\sigma} JS + \frac{1}{4} J^2 \frac{(1 - z_{\sigma}) S G_{1-\sigma}(E - \frac{1}{2} z_{\sigma} JS)}{1 - \frac{1}{2} J G_{1-\sigma}(E - \frac{1}{2} z_{\sigma} JS)}, \end{aligned} \quad (26)$$

$$\begin{aligned} \Sigma_{\mathbf{k}\sigma}^{(n=2)}(E) &\equiv \Sigma_{\sigma}^{(2)(n=2)}(E) \\ &= -\frac{1}{2} z_{\sigma} JS + \frac{1}{4} J^2 \frac{(1 + z_{\sigma}) S G_{2-\sigma}(E - \frac{1}{2} z_{\sigma} JS)}{1 + \frac{1}{2} J G_{2-\sigma}(E - \frac{1}{2} z_{\sigma} JS)}. \end{aligned} \quad (27)$$

E. Weak-coupling behaviour

Since conventional diagrammatic perturbation theory for the KLM is impossible due to the lack of Wick's theorem we determine the weak-coupling behaviour by use of the projection-operator method.^{27,28} Strictly applying the Mori-formalism to the effective-medium KLM yields up to terms J^2 :²⁹

$$\begin{aligned} \Sigma_{\mathbf{k}\sigma}^{s.o.}(E) = & -\frac{1}{2}Jm_\sigma - \frac{1}{4}J^2m_\sigma^2G_{\mathbf{k}\sigma}^{(0)}(E) \\ & + \frac{J^2}{4N^2} \sum_{\mathbf{q}} \left[\langle S_{-\mathbf{q}}^z S_{\mathbf{q}}^z \rangle G_{\mathbf{k}+\mathbf{q}\sigma}^{(0)}(E) \right. \\ & \left. + \left(\langle S_{-\mathbf{q}}^\sigma S_{\mathbf{q}}^\sigma \rangle + 2z_\sigma \langle S_{\mathbf{0}}^z \rangle \langle n_{\mathbf{k}+\mathbf{q}-\sigma} \rangle^{(0)} \right) G_{\mathbf{k}+\mathbf{q}-\sigma}^{(0)}(E) \right]. \end{aligned} \quad (28)$$

The \mathbf{q} -dependent spin operator is defined as usual:

$$S_{\mathbf{q}}^\alpha = \sum_i S_i^\alpha e^{-i\mathbf{q}\mathbf{R}_i}, \quad (29)$$

($\alpha=+, -, z$). $G_{\mathbf{k}\sigma}^{(0)}(E)$ is the effective medium Green function (17) in case of a vanishing self-energy. In the following we are mainly interested in the local self-energy,

$$\Sigma_\sigma(E) = \frac{1}{N} \sum_{\mathbf{k}} \Sigma_{\mathbf{k}\sigma}(E), \quad (30)$$

for which the self-energy (28) further simplifies.

F. High-energy expansion

The spectral moments $M_{\mathbf{k}\sigma}^{(n)}$ of the spectral density (10),

$$M_{\mathbf{k}\sigma}^{(n)} = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE E^n S_{\mathbf{k}\sigma}(E), \quad (31)$$

can be of great importance for testing or constructing unavoidable approximations. This is due to the fact that in principle, the moments can be calculated rigorously and independently of the required spectral density:

$$M_{\mathbf{k}\sigma}^{(n)} = \left[\left(i\hbar \frac{\partial}{\partial t} \right)^n \left\langle \left[c_{\mathbf{k}\sigma}(t), c_{\mathbf{k}\sigma}^\dagger(t') \right]_+ \right\rangle \right]_{t=t'}, \quad (n = 0, 1, 2, \dots) \quad (32)$$

There is a close connection between the moments and the high-energy behaviour of the Green function:

$$G_{\mathbf{k}\sigma}(E) = \int_{-\infty}^{+\infty} \frac{S_{\mathbf{k}\sigma}(E')}{E - E'} = \hbar \sum_{n=0}^{\infty} \frac{M_{\mathbf{k}\sigma}^{(n)}}{E^{n+1}}. \quad (33)$$

This transfers to the self-energy via the Dyson equation:

$$\Sigma_{\mathbf{k}\sigma}(E) = \sum_{m=0}^{\infty} \frac{C_{\mathbf{k}\sigma}^{(m)}}{E^m}. \quad (34)$$

The coefficients $C_{\mathbf{k}\sigma}^{(m)}$ are simple functions of the moments up to order $m+1$.²¹ In the limits $n \rightarrow 0$ and $n \rightarrow 2$, respectively, we can write down corresponding formulas for the partial self-energies in Eq. (18), which we use in the next section to fix free parameters in our basic self-energy ansatz.

III. INTERPOLATING SELF-ENERGY ANSATZ

We want to develop a self-energy approach which fulfills a maximum number of exactly known limiting cases. So the zero-bandwidth case (21), (22) should correctly be reproduced for all temperatures T , band occupations n , and coupling strengths J . Furthermore, the non-trivial results (26), (27) for ferromagnetic saturation, valid for arbitrary bandwidths and couplings, are strong criteria for the self-energy approach. In addition we have the result (28) for the weak-coupling regime holding for all bandwidths and temperatures. All these exact facts can be covered by the following structures of the partial self-energies:

$$\Sigma_\sigma^{(1)}(E) = -\frac{1}{2}JX_{-\sigma} + \frac{1}{4}J^2 \frac{a_{-\sigma}G_{1-\sigma}(E - \frac{1}{2}JX_{-\sigma})}{1 - b_{-\sigma}G_{1-\sigma}(E - \frac{1}{2}JX_{-\sigma})}, \quad (35)$$

$$\Sigma_\sigma^{(2)}(E) = \frac{1}{2}JY_{-\sigma} + \frac{1}{4}J^2 \frac{\hat{a}_{-\sigma}G_{2-\sigma}(E + \frac{1}{2}JY_{-\sigma})}{1 + \hat{b}_{-\sigma}G_{2-\sigma}(E + \frac{1}{2}JY_{-\sigma})}. \quad (36)$$

Here we have assumed for simplicity a local, i.e. \mathbf{k} -independent self-energy, as is the case for all our above-listed exact limiting cases. This assumption is not necessary, but makes some steps of the evaluation easier and a bit more transparent. X_σ and Y_σ are defined in (23), the effective medium propagators $G_{i\sigma}(E)$ in (25).

Equations (35) and (36) contain not yet fixed parameters a_σ , b_σ , \hat{a}_σ , and \hat{b}_σ . They can be derived by use of the high-energy expression (34). In order to do so for the general case, we have to determine four unknown parameters, requiring the first five terms in the expansion (34). On the other hand, for the determination of $C_{\mathbf{k}\sigma}^{(m)}$ for $m=0,1,\dots,4$, the derivation of the first six spectral moments is needed. This turns out to be impossible, in particular because higher (mixed) correlation functions appear in the moments of order $n \geq 3$, which cannot be determined self-consistently. However, simplifications show up in the limits $n \rightarrow 0$ and $n \rightarrow 2$, for which we can separately inspect the partial self-energies needing only the first four moments for, respectively, the empty and the occupied band.

Because of the local character of the partial self-energies $\Sigma_\sigma^{(1,2)}(E)$ we need the local self-energy coefficients:

$$C_\sigma^{(m)} = \frac{1}{N} \sum_{\mathbf{k}} C_{\mathbf{k}\sigma}^{(m)}. \quad (37)$$

A tedious but straightforward calculation eventually yields for the unknown parameters in (35) and (36):

$$a_\sigma = S(S+1) - X_\sigma(X_\sigma + 1), \quad (38)$$

$$\hat{a}_\sigma = S(S+1) - Y_\sigma(Y_\sigma + 1), \quad (39)$$

$$b_\sigma = \hat{b}_\sigma = \frac{1}{2}J. \quad (40)$$

It is easy to check that all the rigorous limiting cases we listed up before, are strictly fulfilled by the now complete result for the self-energy. Eqs. (13) to (18), (23), (24), (35), (36), and (38) to (40) build a close system of equations that can be solved self-consistently for the CKLM as soon as we can express the correlation functions n_σ and Δ_σ by the single-electron Green function (17). This is no problem for n_σ because we can use the spectral theorem to get:

$$n_\sigma = -\frac{1}{\pi N} \sum_{\mathbf{k}} \sum_{i=1}^2 \int_{-\infty}^{+\infty} dE f_{-}(E) \text{Im} G_{\mathbf{k}\sigma}^{(i)}(E - \mu), \quad (41)$$

where $f_{-}(E) = (1 + e^{\beta(E-\mu)})^{-1}$ denotes the Fermi function. Even the mixed correlation function Δ_σ , defined in (24), can rigorously be expressed by $G_{\mathbf{k}\sigma}(E)$. Using the spectral theorem for higher Green functions, properly defined with respect to the two terms of Δ_σ in (24), and exploiting the equation of motion of $G_{\mathbf{k}\sigma}(E)$, one gets:

$$\Delta_\sigma = \frac{2}{NJ\pi} \sum_{\mathbf{k}} \sum_{i=1}^2 \int_{-\infty}^{+\infty} dE f_{-}(E) [E - T_{i\sigma}(\mathbf{k})] \times \text{Im} G_{\mathbf{k}\sigma}^{(i)}(E - \mu). \quad (42)$$

The local moment magnetization $\langle S^z \rangle$ shall be considered as an external parameter being responsible for the induced temperature-dependence of the band states.

Once again we want to stress that all the calculations have been done for quantum mechanical spins, which is in contrast to many of the recent works on the KLM.^{8,9,10}

IV. RESULTS

For the presentation of the results of our theory on the CKLM we have chosen an sc-lattice with the respective Bloch density of states (BDOS) in tight-binding approximation.³⁰ For all calculations we have assumed a bandwidth of 1 eV while the center of gravity of the *free* Bloch band defines the energy zero. For all evaluations we have fixed the Coulomb interaction to $U=2$ eV.

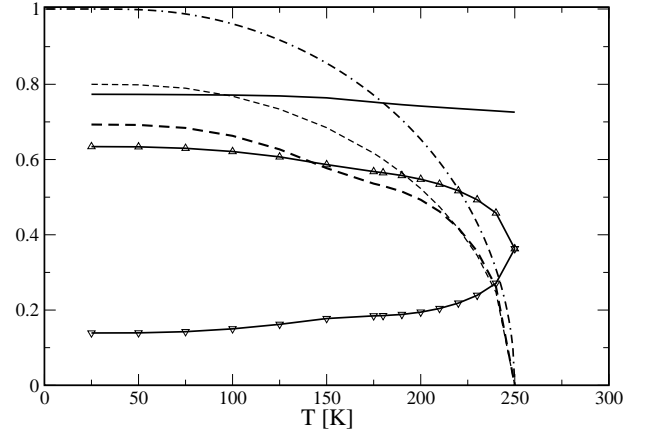


FIG. 1: Temperature dependence of the correlation functions. Dash-dotted line $\langle S^z \rangle / S$, thin dashed line renormalized $\langle S^z \rangle$ [see Eq. (43) and text], thick dashed line electron spin-polarization [see Eq. (44)], Δ -line Δ_\uparrow , ∇ -line Δ_\downarrow , full line $\Delta_\uparrow + \Delta_\downarrow$. Parameters: $S = 3/2$, $n = 0.5$, $U = 2$ eV, $J = 1$ eV, $T_c = 250$ K.

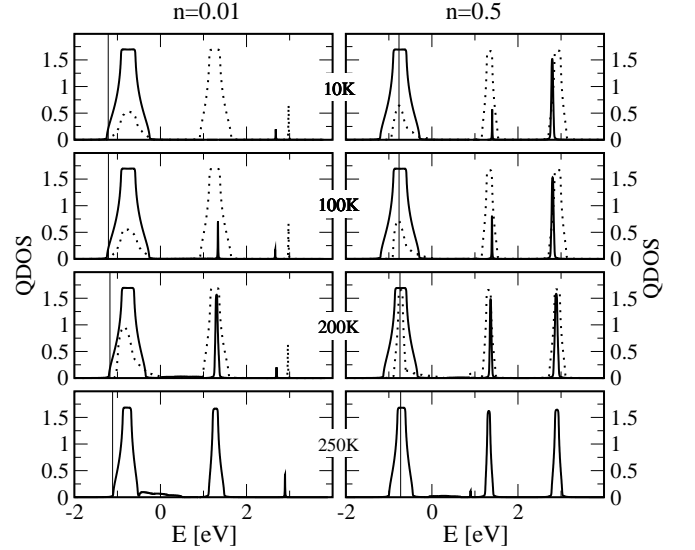


FIG. 2: Quasiparticle density of states for various values of the temperature. Left low-density case, right intermediate band occupation. Full line \uparrow and dotted line \downarrow . Parameters: $S = 3/2$, $U = 2$ eV, $J = 1$ eV. The chemical potential is indicated by a thin vertical line.

Our theory does not aim at a self-consistent determination of the local-moment magnetization^{14,18} but rather at the influence of the interband exchange on the band states. We therefore consider $\langle S^z \rangle$ as a parameter, for which we have chosen a Brillouin function according to the spin value $S=3/2$ with a Curie temperature of $T_c=250$ K (Fig. 1). One has, however, to bear in mind that not all parameter constellations will permit a finite magnetization. Furthermore, saturation $\langle S^z \rangle = S$ may not be reachable by the system in case of finite band occupation due to spin exchange processes. This can be demon-

strated directly by the exact zero-bandwidth solution.²² For in this special case results get unphysical for less than half-filled bands ($n \leq 1$) as soon as

$$\langle S^z \rangle \geq S \cdot \frac{S+1-n}{S+1}. \quad (43)$$

We observe in our theory a similar effect: results may become unphysical when for finite band occupations $\langle S^z \rangle$ exceeds a critical value which depends on n as well as on J/W . For decreasing J/W the *demagnetization factor* becomes smaller, disappearing for $J/W \rightarrow 0$. To bring a certain systematic to our results we have therefore renormalized the parameter *magnetization* $\langle S^z \rangle$ by the factor $\frac{S+1-n}{S+1}$. If we speak in the following of temperature then this is thought to be connected to a magnetization given by a Brillouin function multiplied by this factor. As an example we have plotted in Fig. 1 the renormalized magnetization for $n=0.5$ (thin dashed line).

Figure 2 (left) exhibits the temperature-dependence of the QDOS of the CKLM for the case of a very low band occupation $n=0.01$. $J=1$ eV belongs already to the strong coupling region. The QDOS mainly consists of two subbands for each spin direction. Each of these subbands has a clear physical meaning. Roughly speaking, in the lower (upper) band the electron has oriented its spin parallel (antiparallel) to the localized spin. The distance of the centers of gravity of the subbands is close to $\frac{1}{2}J(2S+1)$ (≈ 2 eV), corresponding to the distance of the two respective energy levels in the zero-bandwidth limit.²² $T=10$ K means that the spin system is almost ferromagnetically saturated. This is a special case, for which our theory turns out to be exact (Sec. IID). The \uparrow -electron has no chance to exchange its spin with the parallel aligned localized spin system. From the exchange interaction (5) only the Ising-like part works, simply leading to a rigid shift of the total spectrum. The \uparrow -QDOS is identical to the sc-BDOS except for the rigid shift. On the other hand, the \downarrow -electron has two possibilities for a spinflip. It can emit a magnon therewith becoming itself an \uparrow -particle. Such a process can happen only if there are \uparrow -states within reach that the excited \downarrow -electron may occupy after the spinflip caused by the magnon emission. This is the reason why the lower \downarrow -subband, which consists of such *scattering states*, covers exactly the same energy region as $\rho_{\uparrow}(E)$. The \downarrow -electron has a second possibility to exchange its spin. It can polarize its nearest spin neighborhood by repeated magnon emission and reabsorption, thus propagating through the lattice as a dressed particle with a virtual cloud of magnons. We call it then the *magnetic polaron*. It has its analogue in the Fröhlich polaron of lattice dynamics. Such polaron states build up the second subband.

For increasing temperature T (i.e. for decreasing magnetization), the \uparrow -spectrum, too, becomes more complicated. Magnon absorption by a \uparrow -electron is equivalent to magnon emission by the \downarrow -electron, with the only exception that emission is always possible, absorption, however, only if there are magnons available. This is not the

case in ferromagnetic saturation. Consequently the \uparrow -spectrum is then relatively simple. With increasing temperature, however, the two spin spectra become more and more similar, until at T_c the spin asymmetry has disappeared. The quasiparticle splitting remains, though.

Let us now discuss the dependence on the band occupation. In Fig. 3 the QDOS is plotted for various band occupations at $T=10$ K, i.e., for practically maximum local spin magnetization. First of all, we observe the appearance of a third quasiparticle subband due to possible double occupancies of lattice sites, which require the additional Coulomb energy U . According to the exact zero-bandwidth limit one could expect for less than half-filled bands even a second high-energy subband.²² This is not the case because one of the upper bands has a vanishing spectral weight. This fact already holds in the $W=0$ -case. For more than half-filled bands one of the low-energy subbands disappears.

Two details of the occupation dependence of the QDOS are worth to be stressed. First we learn from the n -dependent position of the chemical potential in the ferromagnetic phase (Fig. 3) that the electron system is never completely spin-polarized. This is a natural consequence of the spin exchange processes between itinerant and localized electrons and in contradiction to several other treatments of the KLM.^{10,31} Total spin polarization is only true under the unphysical assumption of classical spins. The second point concerns the polaron band, which for less than half-fillings is never occupied (Fig. 3). The chemical potential is always in the lowest subband reaching its upper edge for $n \rightarrow 1$. At the same moment the polaron band disappears. The chemical potential jumps into the uppermost subband for more than

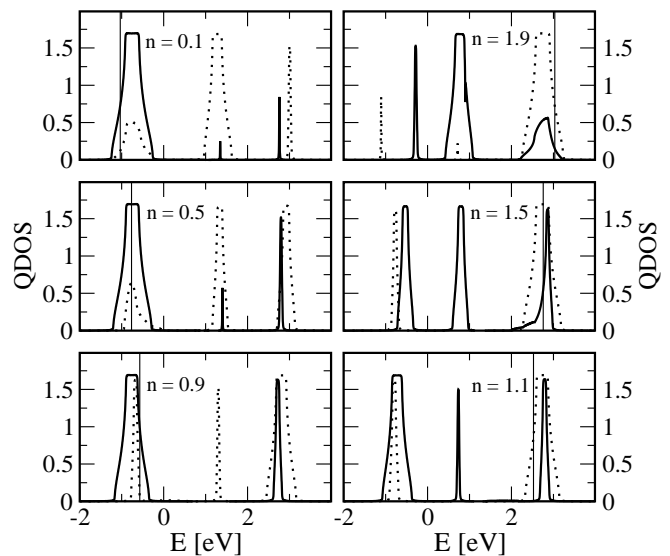


FIG. 3: Quasiparticle density of states for various values of the band occupation (ferromagnetic region). Full line for spin up and dotted line for spin down. Parameters: $S = 3/2$, $U = 2$ eV, $J = 1$ eV, and $T = 10$ K.

half-fillings guaranteeing therewith particle-hole symmetry. Note that the middle band in case of $n>1$ is the polaron band for holes, centred at $U - \frac{1}{2}J(S+1)$.

Figure 4 demonstrates the J -dependence of the (paramagnetic) QDOS for a band filling of $n=0.5$. For weak (moderate) couplings the two lower subbands overlap, separating, however, as soon as J exceeds a critical value. The existence of the two low-energy subbands can roughly be understood from the zero-bandwidth limit. In the strong coupling regime ($JS \gg W$) the band electron has only a low mobility being trapped by the local spin for a rather long time. In such a case the local spin defines the quantization axis. When we speak of *up spin band* or *down spin band* we refer the electron spin to an external axis. However, in the strong coupling regime the relative orientation of the electron spin in the local frame is decisive for the excitation energies. The lowest subbands, up-spin as well as down-spin, consists of states where the excited electron enters directly or after magnon emission (absorption) the local frame parallel to the local spin. If it arrives at the local frame antiparallel to the local spin then it goes into the second low-energy subband centered at $+\frac{1}{2}J(S+1)$. There is a slight probability that the electron is not trapped by the localized spin but rather propagating with high mobility through the spin lattice. Then the total magnetization $\langle S^z \rangle$ will become decisive as effective quantization axis, leading to a mean-field type behaviour of the quasiparticle according to the first term in the self-energy (35). We interpret the small shoulder in between the two lower subbands in Fig. 4 in such a way as already discussed in an earlier work.²¹ This shoulder becomes more and more unimportant with increasing exchange coupling.

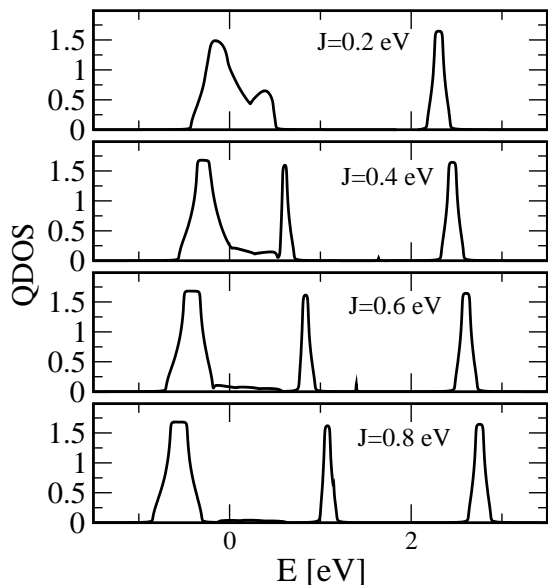


FIG. 4: Quasiparticle density of states for various values of the Hund coupling J . Parameters: $S = 3/2$, $U = 2$ eV, $n = 0.5$, and $T = 250$ K.

Let us now inspect the temperature dependence of the quasiparticle spectrum for a higher band occupation. Figure 2 (right) shows as an example the QDOS for $J=1$ eV and $n=0.5$. The positions of the bands are hardly affected by temperature as one might expect because of the first term in the self-energy (35) and (36), respectively. For strong exchange couplings the second term, which incorporates all the spinflip processes, dominates. As explained just before, the local frame is decisive being of course unaffected by temperature. The temperature determines, however, the probability with which an externally prepared σ -electron enters the local frame as \uparrow -(\downarrow)-electron, and this fixes the spectral weights of (areas under) the subband-DOS. For example, in the ferromagnetically saturated spin system ($T=0$) an \uparrow -electron cannot enter the local frame antiparallel to the localized spin. Therefore the middle subband disappears because of vanishing spectral weight. This changes with increasing temperature, i.e. decreasing magnetization by directional disorder of the local spins. For $T \geq T_c$ the spin asymmetry has disappeared, but there remains a quasiparticle splitting into three peaks, which are all of comparable spectral weights. For strongly coupled Kondo-lattice systems such an unconventional splitting should be observable in a respective photoemission experiment.

Up to now we have only discussed the strong coupling case which we are mainly interested in here. To give an example for weaker couplings we present in Fig. 5 the spectral density (10) for $T = T_c$ and two different exchange couplings J . The low-energy part belongs to scattering states and the magnetic polaron. The high-energy peak is due to double occupancies, fairly uninteresting in the case of a less than half-filled band. For $J=0.2$ eV the polaron peak dips into the scattering spectrum; the quasiparticle therefore gets a finite lifetime. There is a remarkable \mathbf{k} -dependent shift of spectral weight. For a \mathbf{k} -vector from the bottom or from the top of the respective quasiparticle subband the magnetic polaron is rather stable, while experiencing substantial damping in between. In systems with stronger exchange couplings ($J=0.4$ eV) the polaron peak, negligibly damped and hardly dispersive, splits off the scattering part. It contributes to a very narrow quasiparticle subband (see Fig. 4).

By use of Eqs. (41) and (42) we can eventually evaluate the average spin-dependent particle density n_σ and the mixed correlation Δ_σ , and therewith the conduction band polarization,

$$m = \frac{n_\uparrow - n_\downarrow}{n_\uparrow + n_\downarrow}, \quad (44)$$

and the spin scalar product which appears in the exchange Hamiltonian (1):

$$\langle \sigma_i \cdot \mathbf{S}_i \rangle = \Delta_\uparrow + \Delta_\downarrow. \quad (45)$$

A typical example ($J=1$ eV, $n=0.5$) is plotted in Fig. 1. We recognize that even for strong couplings the electron spin polarization is far from being complete. No

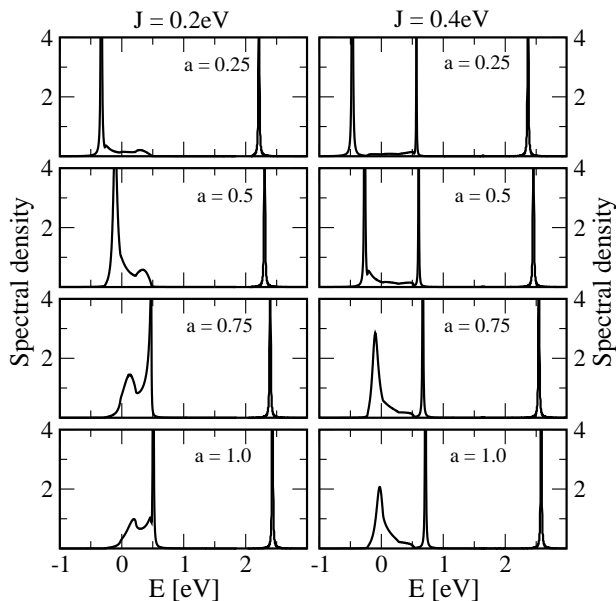


FIG. 5: Spectral density for two values of J and three values of \mathbf{k} along the (a, a, a) -direction. Parameters: $S = 3/2$, $U = 2$ eV, $n = 0.5$, and $T = 250$ K.

more than 70% polarization are observed. This again strongly contradicts other treatments of the KLM.^{10,31} The higher correlation functions Δ_{\uparrow} and Δ_{\downarrow} exhibit a distinct temperature-dependence, while the sum of both makes the spin-spin scalar product (45) almost temperature-independent.

V. CONCLUSIONS

We have presented an interpolating self-energy approach to the many-body problem of the *correlated Kondo-lattice model* which interpolates between a maximum number of rigorous statements and exact limiting cases of the (in general) not exactly solvable model. Correlations between the band electrons are accounted for by an on-site Coulomb interaction of Hubbard type. In this paper we were not interested in the investigation of how the band electron correlations effect the magnetic stability within the KLM, as was done, for instance, in Ref. 10. A corresponding study of the (self-consistent)

magnetic part is currently being done and will be presented at a later stage. Here the mentioned correlations simply help to avoid unphysical double occupancies of lattice sites as energetically favored excitations and to separate respective quasiparticle subbands.

In our theory the strongly exchange coupled system is accounted for by the exact zero-bandwidth limit for all temperatures and band occupations. The weakly coupled system is addressed by second order perturbation theory (projection-operator technique) for all temperatures and bandwidths. For further interpolation between the limits we used the exact but non-trivial results for the special case of a single electron (hole) in an otherwise empty (fully occupied) band interacting with a ferromagnetically saturated spin system. This special case exhibits practically all typical elementary processes that determine the physics of the CKLM. It holds for all coupling strengths and bandwidths. Finally we guaranteed the correctness of spectral moments via fitting free parameters in the self-energy ansatz.

The energy spectra show strong dependencies on temperature and band occupation, particularly in the strongly exchange coupled regime which is thought to be relevant for the *colossal magnetoresistance materials* as well as for manganese-doped GaAs (*spintronics*). In our opinion the results clearly demonstrate the importance to retain the quantum nature of the localized spins. To replace them, for technical reasons, by classical spins appears to be inadequate.

It must be considered as a shortcoming of the approach that the local moment magnetization had to come into play only as an external parameter, which can give rise to certain inconsistencies. It is planned for the future to incorporate the local moment system into the self-consistency circle.

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